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Joan H. Novak
Atmospheric Sciences Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

ATMOSPHERIC SCIENCES RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

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ABSTRACT

A comprehensive Regional Acid Deposition Model (RADM) is being developed and a simpler fast-turn-around "engineering" model(s) (EM) is being designed by the National Center for Atmospheric Research as part of the National Acid Precipitation Assessment Program (NAPAP). This paper describes how potential assessment applications and research questions affect those model designs and the subsequent emission inventory requirements. Finally a recommendation is made for EPA to consolidate inventory development efforts to produce an agency emission inventory applicable to the wide spectrum of models and applications throughout EPA.

INTRODUCTION

The scope and complexities of the acid rain issue in the United States present modelers with conflicting requirements. The models are expected to be accurate and scientifically credible as well as easy to use for assessment purposes. Task Group C of NAPAP - Atmospheric Processes - is responsible for coordinating the model development and research efforts. The primary model development activities are being performed at the National Center for Atmospheric Research(NCAR) in Boulder, Colorado. These activities include the development of a comprehensive Regional Acid Deposition Model (RADM) and a simpler fast-turn-around "engineering" model(s). These models have great potential to provide information needed to achieve many of the major goals of NAPAP(1):

- Understand the basic chemical and physical processes related to acid deposition
- Assess the severity of acid deposition effects
- Determine the causes of acid deposition
- Assess the relative importance of different causes of acid deposition
- Assess the effects of man's activities on acid deposition
- Determine effective control strategies

DISCUSSION

The purpose of this discussion is to present an overview of the current modeling approach with special emphasis on emission inventory requirements. The scientific community agrees that a rigorous treatment of processes relevant to acid deposition is essential for credible results. Thus, the RADM will include a comprehensive description of all the major physical and chemical processes currently known to effect acid deposition. However, incorporation of this level of detail on a regional scale extends the model execution time beyond what is considered reasonable to address the policy and assessment questions; these require calculation of long term averages with sufficient speed to permit extensive experimentation with alternative solution strategies.

The EM, therefore, is being specifically designed to address the policy and assessment applications . This model will incorporate condensed representations of several simple nonlinear physical and chemical processes contained in the RADM and consequently will require a relatively short execution time. The credibility of the EM can, at a minimum, be evaluated by comparison with the more accurate RADM results.

Recent reviews(1,2) have shown that a three dimensional Eulerian framework is the most feasible general approach for both RADM and EM. This decision has significant impact on spatial resolution requirements of emissions. The current RADM domain covers the entire continental United States and southern Canada. Theoretical considerations suggest a 20 x 20 km^2 grid resolution, however, due to computer time and space limitations a compromise of 80 x 80 km^2 grid spacing was chosen. A larger grid size may give substantial inaccuracies. Major point source emitters and many urban areas, nevertheless, must be treated individually to determine the impact of specific sources and to correct for the effect of chemical and physical phenomena on a subgrid scale. Within a grid cell, inhomogeneities may exist in emissions, chemical reaction types and rates, deposition, and transport phenomena. Development of an independent module to calculate correction factors for each grid due to these inhomogeneities is being planned. Thus a 20 x 20 km^2 grid resolution for area emissions is required to adequately parameterize the effect of sub-grid scale emission patterns. The RADM has up to 15 vertical layers and can incorporate emissions into each of these layers. Most models assume emission at the surface with instantaneous mixing aloft. Multiple levels of emission should have a definite accuracy advantage, especially near the source.

The RADM because of its size and complexity is typically executed in an episodic mode for a two to three day period. Annual or long term averages can be approximated by the weighted average of representative episodic model results. The RADM typically requires hourly emissions for these episodic applications. A representative weekday/weekend diurnal pattern for each season is adequate to produce the required temporal variation of emissions(3).

A comprehensive chemical reaction scheme detailed enough to handle nonlinearities resulting from sulfur, nitrogen oxide and ozone chemistry, and cloud chemistry in both the gaseous and aqueous phases is necessary to achieve many of the major objectives of NAPAP. An emissions inventory is being developed which is capable of addressing the above issues on the required temporal and spatial time scales. It will include:

- major acid precursors (SO_2,NO_x)
- sulfate aerosols because of their contribution to the total sulfur budget
- volatile organic compounds and carbon monoxide because of their importance in the oxidation process
- reactive hydrocarbons and nitrogen oxides because of their role in oxidant production
- direct sources of acid species such as organic acids, and hydro chloric and hydrofluoric acid whose vapors are incorporated into clouds and precipitation

- coarse aerosols(>2.5μm) and particles important to acid formation
- ammonia for its role as a buffering agent in cloud chemistry
- other buffering aerosol species such as alkaline dust
- aerosol components key to catalytic conversion in aqueous reactions (soot, iron, manganese)
- naturally emitted precursors to acid rain such as reduced sulfur species
- other naturally emitted species related to acid or oxidant formation

In contrast emission requirements for the EM are less stringent. The model domain remains the same as RADM, however, grid resolution may be reduced. The EM will have only 3 to 5 vertical levels and each specific version would treat only one family of chemical species. Parameterization of transformation and deposition processes would include simplifications of the nonlinear chemistry based on knowledge gained from RADM executions and observation data(2). Therefore emission species requirements and, in fact, all other emission requirements are easily satisfied by the RADM emissions dataset.

CONCLUSIONS

The goals of the NAPAP are too broad to rely on a singular solution. This brief overview of the atmospheric modeling approach illustrates the conflicting demands of the research and assessment applications and their implications for emissions inventory development. The inventory developers must provide an emissions database at a level of resolution that meets the most stringent requirements, and yet be flexible enough to transform those base emissions into appropriate spatial, temporal, and species resolutions to satisfy the full spectrum of needs of the scientific and assessment/policy communities. They must also be able to provide estimates of uncertainty associated with the emissions.

Finally, acid rain is only one of the many air pollution problems facing EPA today. Modeling assessment of other problems such as ozone, sulfate, visibility, particulate, etc. have many of the same basic emission inventory requirements even though differences do exist. I recommend that EPA integrate emission inventory development activities to provide an agency inventory that will satisfy the various emission requirements of current and anticipated modeling and assessment programs.

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